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Quantitative Computer Representation of Propellant Processing

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With the technology currently available for the manufacture of propellants, it is possible to control the variance of the total specific impulse obtained from the rocket boosters to within approximately 5%. Though at first inspection this may appear to be a reasonable amount of control, when we consider that any uncertainty in the total kinetic energy delivered to the spacecraft translates into a design with less total usable payload, even this degree of uncertainty becomes unacceptable. There is strong motivation to control the variance in the specific impulse of the shuttle's solid boosters. Any small gains in the predictability and reliability of the boosters would lead to a very substantial payoff in Earth-to-orbit payload. The purpose of this study is to examine one aspect of the manufacture of solid propellants, namely, the mixing process. We attempt to introduce a unique methodology to enable understanding of this process.

The traditional approach of computational fluid mechanics is notoriously complex and time consuming. We wish to make certain simplifications, yet be able to investigate certain fundamental aspects of the mixing process as a whole. It is possible to consider a mixing process in a mathematical sense as an operator, F , which maps a domain back upon itself (Figure 1.9). An operator which demonstrates good mixing should be able to spread any subset of the domain completely and evenly throughout the whole domain by successive applications of the mixing operator, F .

A two-dimensional model was first developed using this approach. The differential equations of motion were designed to satisfy conditions of continuity and incompressibility for two-dimensional flow in a unit circle. These equations of motion were designed by Arthur Maser and are given as:

$$\begin{aligned} \dot{x} = & [1 + \sin(t)] \left\{ \frac{2y[4x - 2 + [(2 - x)^2 - 3(1 - x^2 - y^2)]^{1/2}]}{3[(2 - x)^2 - 3(1 - x^2 - y^2)]^{1/2}} + 2y \right\} \\ & + [1 - \sin(t)] \left\{ \frac{2y[4x + 2 - [(2 + x)^2 - 3(1 - x^2 - y^2)]^{1/2}]}{3[(2 + x)^2 - 3(1 - x^2 - y^2)]^{1/2}} + 2y \right\} \end{aligned} \quad (1)$$

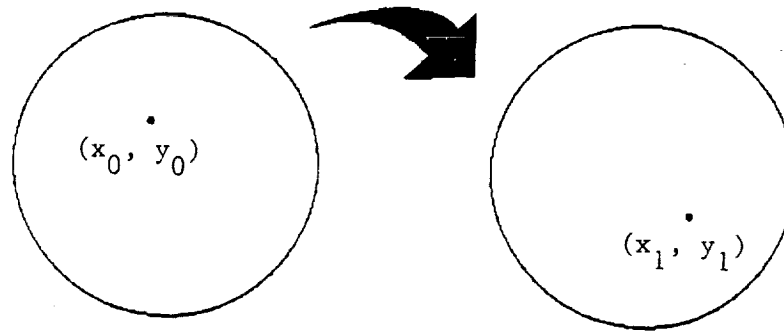


Figure 1.9 Application of mixing operator in a two-dimensional domain.

$$\begin{aligned}
 \dot{y} = & [1 + \sin(t)] \left\{ \frac{2}{9} \left[2x - 2 - [(2 - x)^2 - 3(1 - x^2 - y^2)]^{1/2} \right] \right. \\
 & \times \left[2 + \frac{4x - 2}{[(2 - x)^2 - 3(1 - x^2 - y^2)]^{1/2}} \right] \Bigg\} \\
 & + [1 - \sin(t)] \left\{ \frac{2}{9} \left[2x - 2 + [(2 + x)^2 - 3(1 - x^2 - y^2)]^{1/2} \right] \right. \\
 & \times \left[4 + \frac{4x - 2}{[(2 + x)^2 - 3(1 - x^2 - y^2)]^{1/2}} \right] \Bigg\}.
 \end{aligned} \tag{2}$$

If we examine the streamlines generated by this velocity function, we can see that the flow consists of two superimposed eccentric vortices, rotating in opposite directions. The two vortices lie along the x -axis at $x \pm 0.5$. The two components of the flow are modulated by sinusoidal forcing functions that are 180° out of phase. It is the periodic forcing function that gives rise to the chaotic behavior of the flow by perturbing the regular flow field set up by the nested eccentric vortices. Equation (1) is therefore an attempt to design a mapping that will give random mixing from completely nonrandom functions.

Numerical methods were employed to investigate these equations in order to determine if they can give rise to mixing. The computational process and the animation of the results were conducted on a Silicone Graphics IRIS workstation. One objective was to determine if any small region within the domain can spread itself more or less evenly throughout the whole domain given sufficient applications of the mixing operator. To demonstrate this, we defined small clusters of points within the

domain and integrated the equations of motion with the initial conditions being the starting locations of each of these particles. The path of each individual particle could then be followed across successive iterations of the mixing cycle. The period of the mixing cycle is defined as the period of the sinusoidal forcing functions. This approach mimics a traditional approach for studying flow fields.

In laboratory experiments, highly localized amounts of tracer dyes are introduced, via injection, into the fluid, and the position and the distribution of these dyes can be followed as the flow develops. In the numerical experiment, each group or species of particles is branded with its own particular color so that the species can be followed throughout the experiment and its interaction with other species can be studied visually. To be consistent with the mapping approach, the position of each of the particles was updated after each completion of a mixing cycle. In several simulations of the mixing process, five sets of particles, initially very tightly spaced together, were considered. Each block of particles represents a 30-by-30 set of particles, and we ran the simulations across 20 iterations of the mixing cycle. Figure 1.10 documents the graphical animation derived for these simulations. Each successive frame in the sequence represents the application of one or more mapping operations onto the previous frame and, thus, we are able to study how the flow field evolves through time. We can see how very quickly all apparent structure to the species distribution becomes lost, and we state that our original mapping can give rise to good mixing of the domain within a few iterations of the mixing cycle. We recall a theorem in set theory that states that for any two-dimensional mapping of a domain back upon itself, there must be at least one invariant set or, in terms of the mixing process, at least one dead zone. We therefore seek to find this invariant set. If we animate the same data set such that each successive mapping of the species is superimposed on top of the previous ones, then any region of the domain that remains unmixed should become apparent. We find that when we graph the data with this approach, one dead zone can be found in the lower right-hand corner (Figure 1.11).

Another test of mixing can be outlined as follows. We partition the domain into many elements of equal area. We begin with a particle in some initial position within the domain and follow the particle as it takes many cycles through the mixing operator. A measure can be defined as the number of times the particle falls within an element divided by the total number of iterations. A necessary but not sufficient condition for perfect mixing is that this measure must go to a mean value for each partition as the number of iterations becomes very large. When we apply this test to our operator, we can see that the invariant set becomes apparent as a trough in the plot of the density function (Figure 1.12).

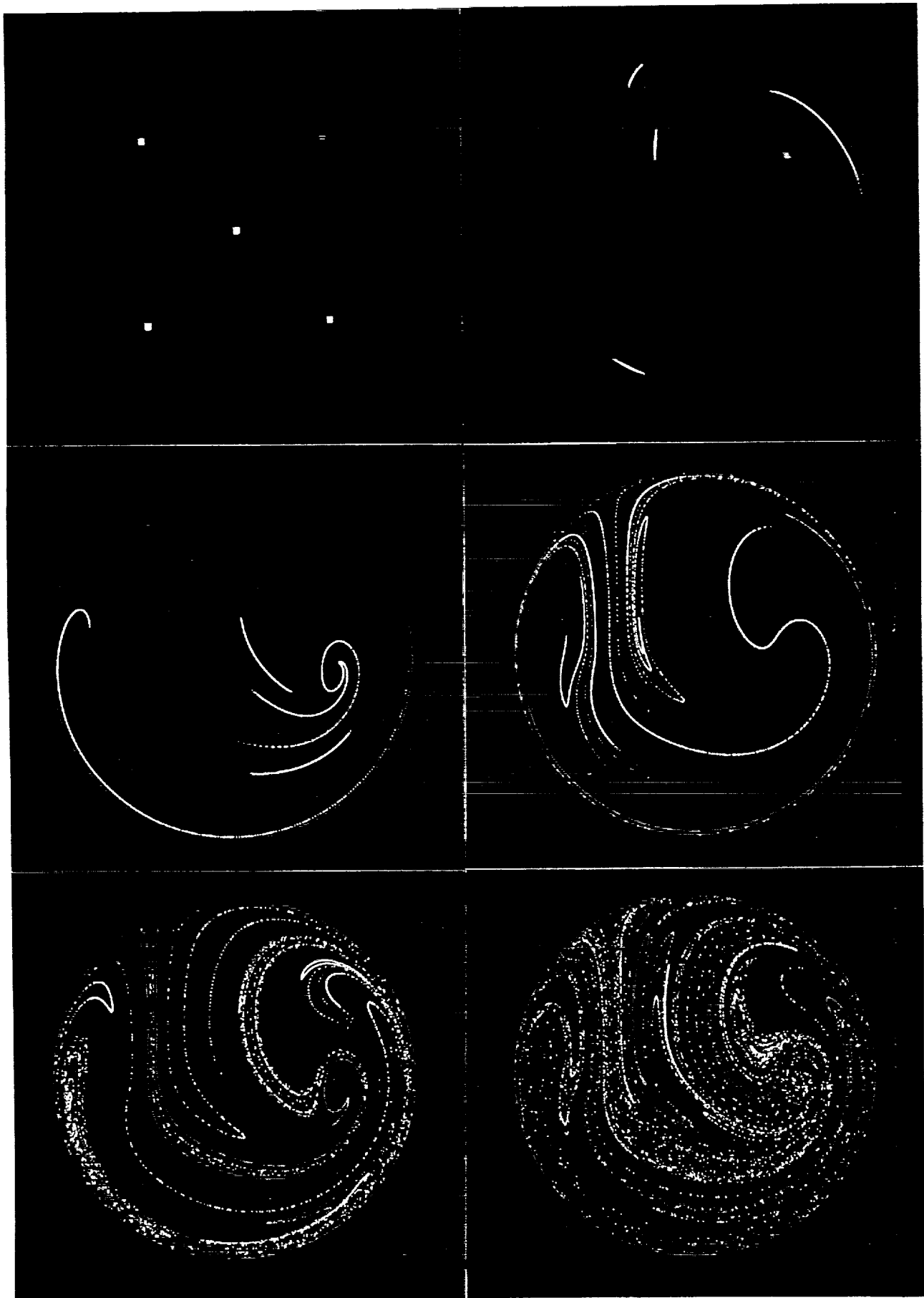
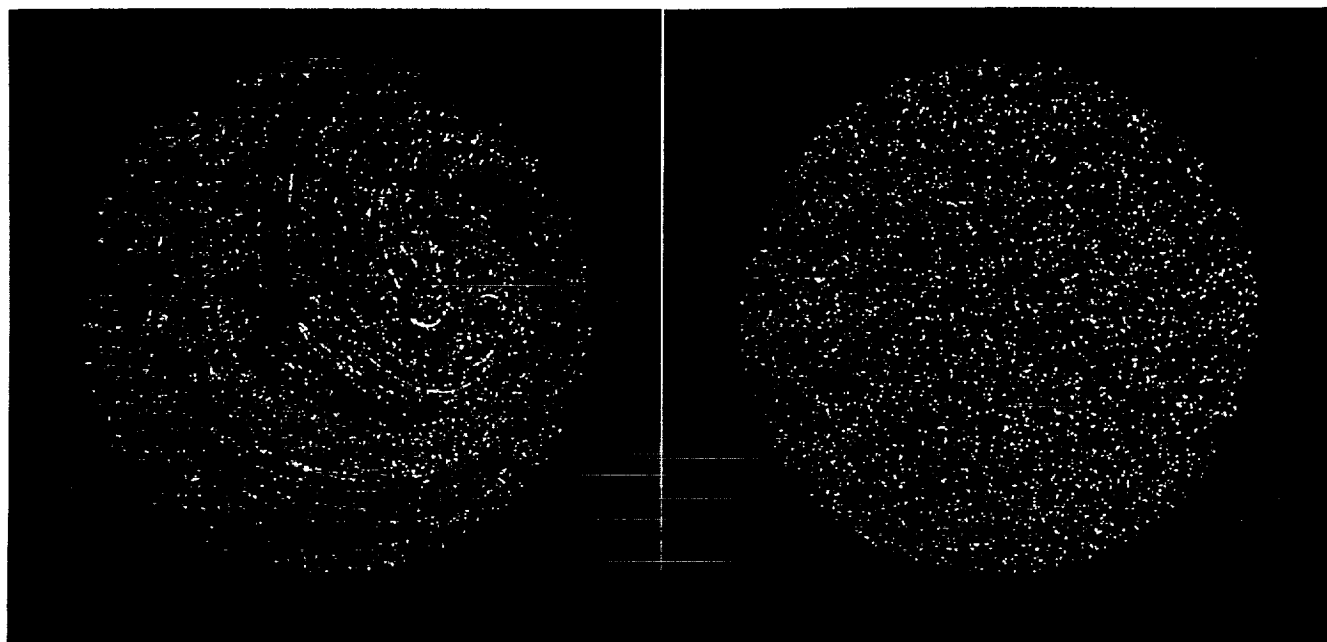


Figure 1.10 Graphical visualization of a two-dimensional mixing process.

Figure 1.10 (Continued).



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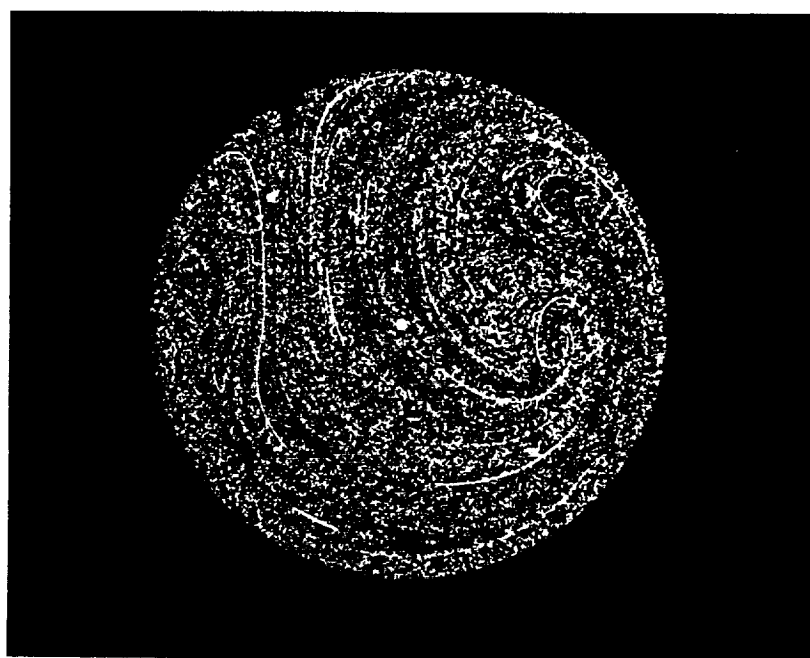


Figure 1.11 Two-dimensional model after 20 iterations.

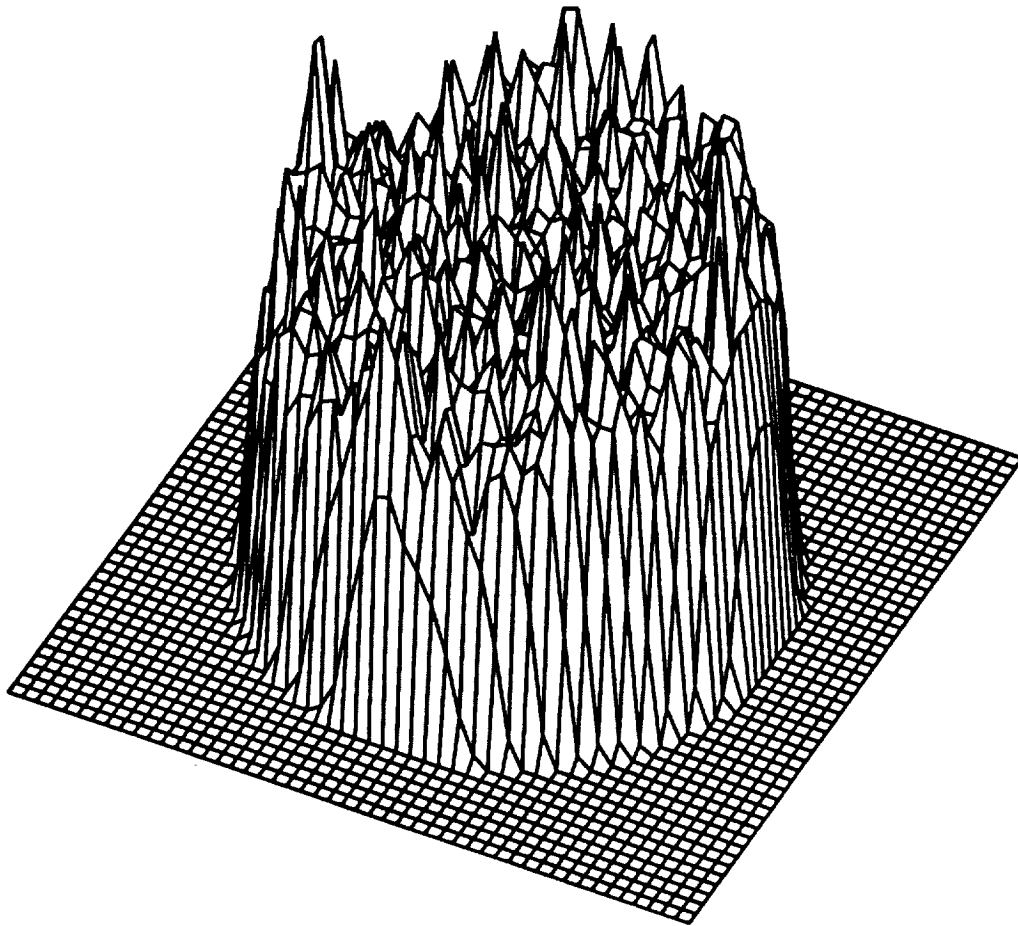


Figure 1.12 Probability density function for two-dimensional mapping.

Later work expanded this approach to investigate mixing in three dimensions. Here, the domain was a torus that was cut and mapped to a unit cube. Particles would flow across the domain and, upon impinging upon the boundary, would be mapped to a point on the opposite face. The mapping function chosen for this experiment was the well-known Baker's transformation. This transformation is an example of a discontinuous mapping that can be used to investigate mixing due to its action of stretching and folding a domain back upon itself (Figure 1.13). We are guaranteed ergodicity through successive iterations of the mapping due to its discontinuity. Real mixers can be designed to mimic this action of splitting, stretching, and refolding the flow without the traditional use of paddles. As in the two-dimensional case, an initially small, very tightly spaced group of particles was carried along by the flow field and the graphical visualization of the results showed the presence of mixing (Figure 1.14). In the three-dimensional case, it was also observed that pseudorandom behavior can be induced from completely nonrandom functions.

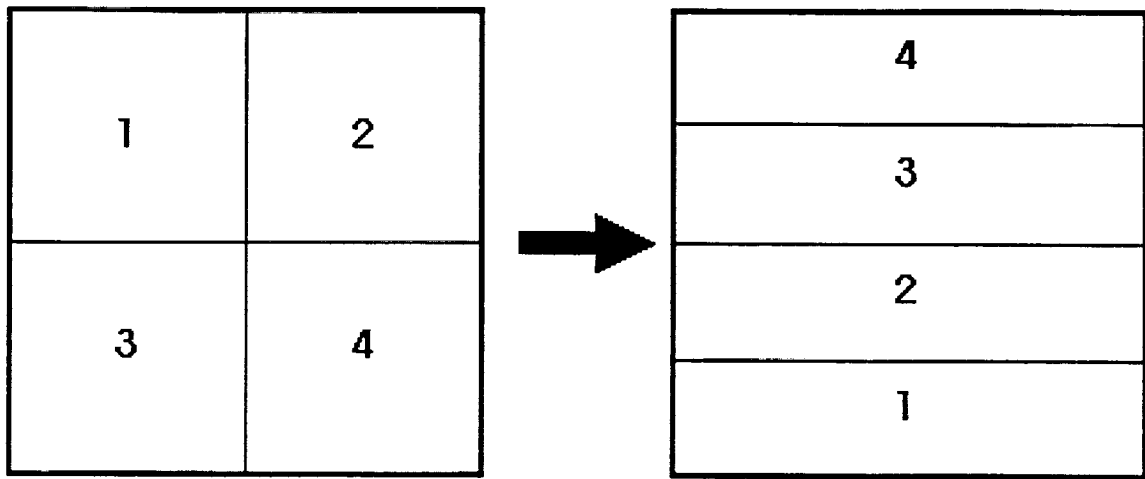


Figure 1.13 Baker's transformation in base two.

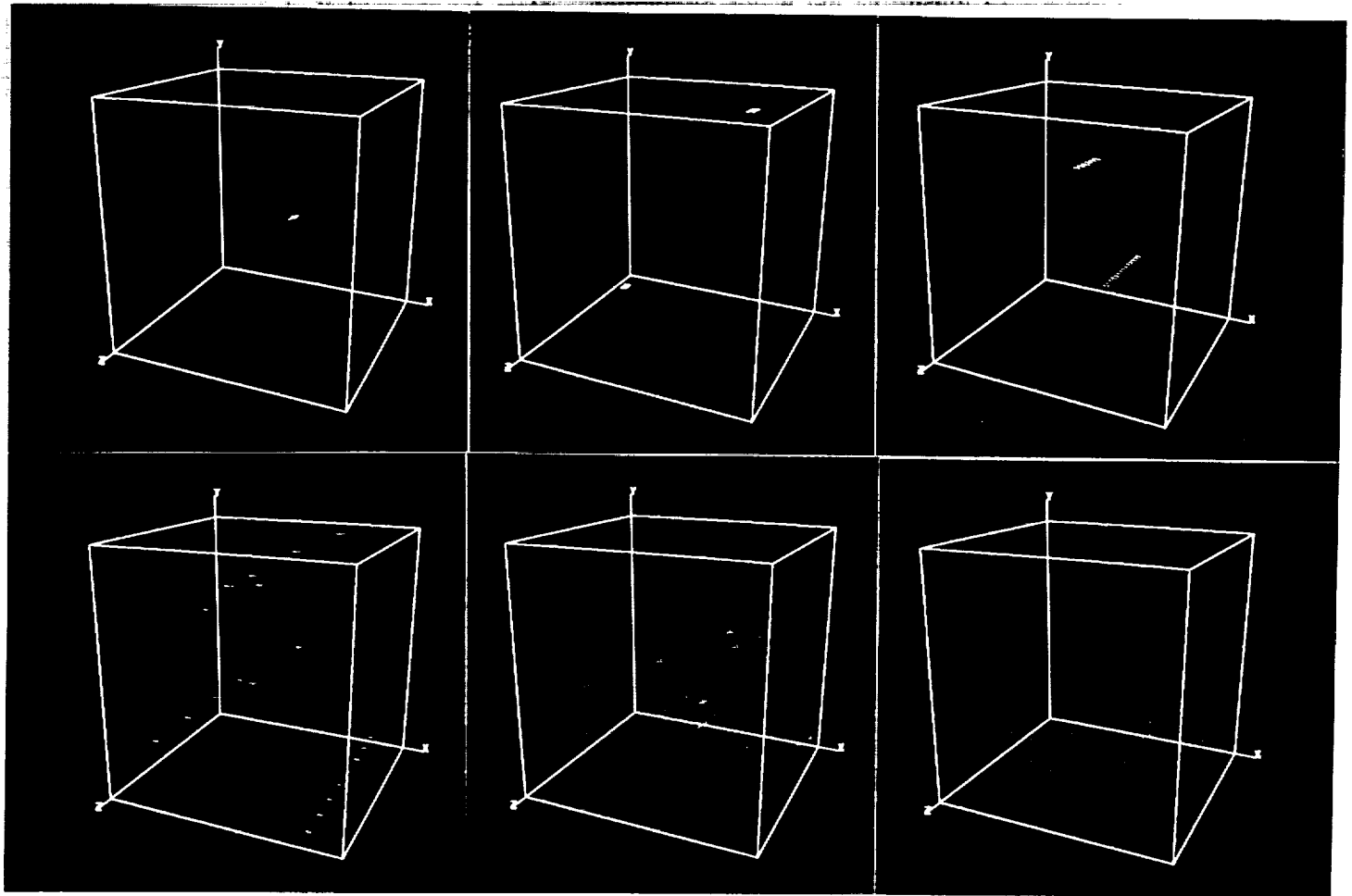


Figure 1.14 Graphical visualization of three-dimensional mixing process.